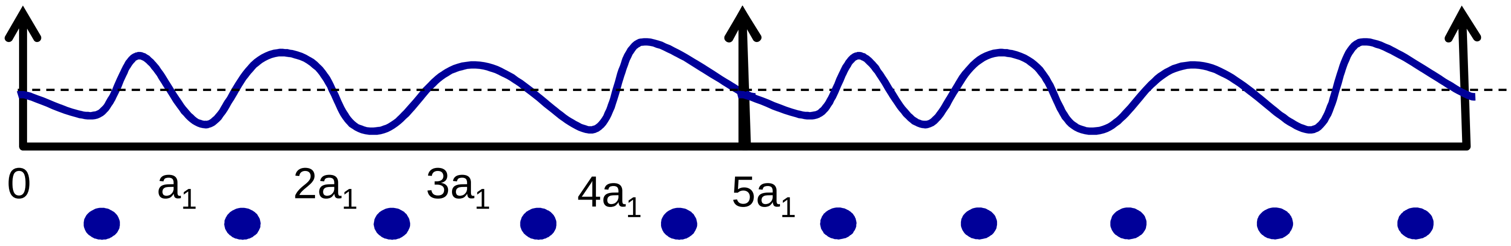
Condições de contorno de Born-von Karman

- Tamanho do sistema = número de células primitivas:

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$



$$\phi_{\mathbf{k}}(\mathbf{r}) = A e^{i\mathbf{k}\cdot\mathbf{r}}$$

Tamanho do sistema:

$$\mathbf{L} = N_1\mathbf{a}_1 + N_2\mathbf{a}_2 + N_3\mathbf{a}_3$$

Volume da célula primitiva: $V_{\mathbf{r}}^{\text{cell}} = (\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)$

Volume do sistema: $V_{\mathbf{r}} = N_1 N_2 N_3 V_{\mathbf{r}}^{\text{cell}}$

Condições periódicas de contorno:

$$\phi(\mathbf{r}+\mathbf{L}) = \phi(\mathbf{r}) \Rightarrow e^{i\sum_j N_j \mathbf{a}_j\cdot\mathbf{k}} = 1$$

$$\mathbf{a}_\ell \cdot \mathbf{A}_j = 2\pi\delta_{\ell j}$$

Quantização de **k**:

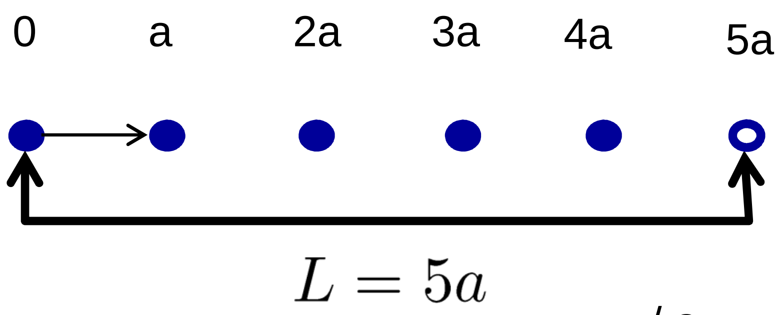
$$\mathbf{k} = \sum_{j=1}^{3} \frac{m_j}{N_j}\mathbf{A}_j$$

Volume ocupado por cada estado no espaço **k**:

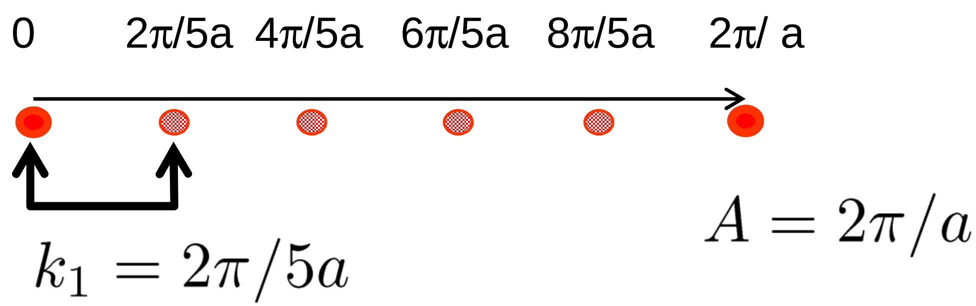
$$V_{\mathbf{k}}^{\text{1st}} = \frac{\mathbf{A}_1}{N_1} \cdot \frac{\mathbf{A}_2}{N_2} \times \frac{\mathbf{A}_3}{N_3} = \frac{1}{N}\mathbf{A}_1 \cdot \mathbf{A}_2 \times \mathbf{A}_3$$

Exemplo: rede 1D

- Rede direta (N=5):



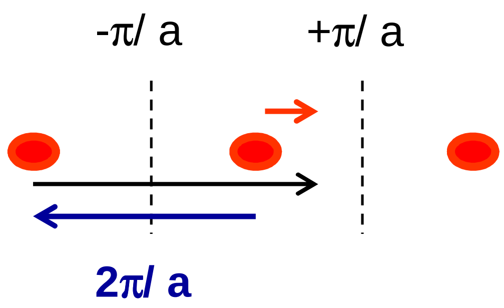
- Rede recíproca: $\mathbf{a}_1 \cdot \mathbf{A}_1 = 2\pi$



- 1a Zona de Brillouin:

$$k = q - G$$

$$-\frac{\pi}{a} \leq q \leq +\frac{\pi}{a}$$

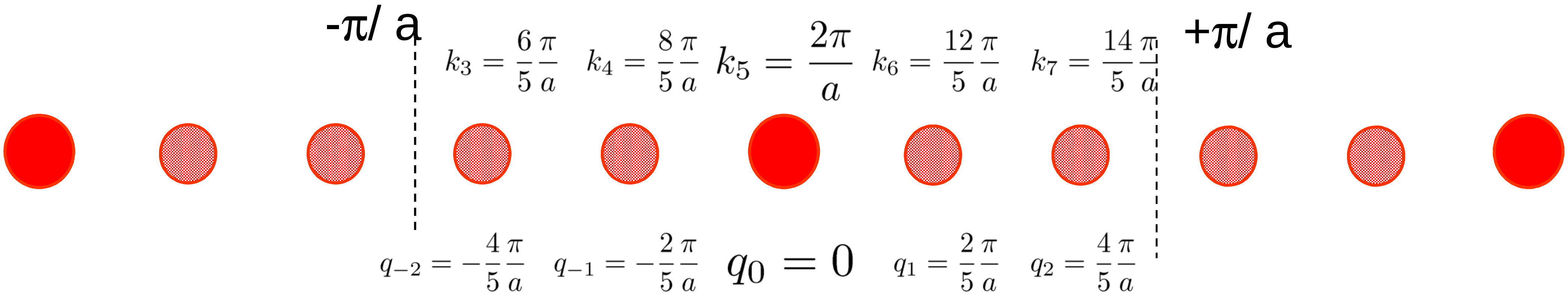


- Quantização de k e q:

$$k_m = \frac{m}{N}\left(\frac{2\pi}{a}\right)$$

$$q_{m'} = \frac{2m'}{N}\left(\frac{\pi}{a}\right)$$

$$|2m'| \leq N$$



Eq. de Schrödinger em um potencial periódico

- Eq. de Schrödinger:

$$\left[-\frac{\hbar^2}{2m^*}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r}) = \varepsilon\Psi(\mathbf{r})$$

Solução (ondas planas):

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} \mathcal{C}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \qquad \mathbf{k} = \sum_{j=1}^{3} \frac{m_j}{N_j}\mathbf{A}_j$$

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{r}\cdot\mathbf{G}}$$

$$\mathbf{G} = m_1\mathbf{A}_1 + m_2\mathbf{A}_2 + m_3\mathbf{A}_3$$

- Substituindo na Eq. de Schrodinger (Tarefa):

$$\boxed{\left(\frac{\hbar^2 k^2}{2m^*} - \varepsilon\right)\mathcal{C}_{\mathbf{k}} + \sum_{\mathbf{G}} V_{\mathbf{G}}\mathcal{C}_{\mathbf{k}-\mathbf{G}} = 0}$$

- Escrevendo em termos de um vetor **q** na 1a ZB (Tarefa): $\mathbf{k} = \mathbf{q} - \mathbf{G}'$

$$\left(\frac{\hbar^2(\mathbf{q}-\mathbf{G}')^2}{2m^*} - \varepsilon\right)\mathcal{C}_{\mathbf{q}-\mathbf{G}'} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}'}\mathcal{C}_{\mathbf{q}-\mathbf{G}''} = 0$$

Equação de auto-valores ε(**q**).
Note que ε(**q**)=ε(**q**+**G**)!!

Teorema de Bloch

$$\Psi(\mathbf{r}) = \sum_{\mathbf{k}} \mathcal{C}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

Equação para os coeficientes:

$$\left(\frac{\hbar^2(\mathbf{q}-\mathbf{G}')^2}{2m^*} - \varepsilon \right) \mathcal{C}_{\mathbf{q}-\mathbf{G}'} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}'} \mathcal{C}_{\mathbf{q}-\mathbf{G}''} = 0$$

- Soluções da Eq. de Schrodinger: $\Psi_{\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{G}} \mathcal{C}_{\mathbf{q}-\mathbf{G}} e^{i(\mathbf{q}-\mathbf{G})\cdot\mathbf{r}}$

$$\Psi_{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \left(\sum_{\mathbf{G}} \mathcal{C}_{\mathbf{q}-\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} \right) \equiv e^{i\mathbf{q}\cdot\mathbf{r}} u_{\mathbf{q}}(\mathbf{r})$$

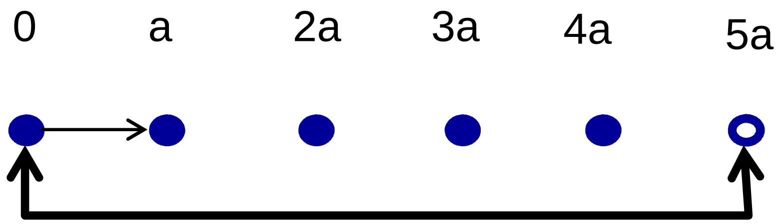
- Teorema de Bloch: as soluções da Eq. de Schroedinger podem ser escritas na forma:

$$\boxed{\Psi_{\mathbf{q}}^{(j)}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} u_{j,\mathbf{q}}(\mathbf{r})}$$

onde $u_{j,\mathbf{q}}(\mathbf{r})$é uma função periódica (com mesmo período do potencial): $u_{j,\mathbf{q}}(\mathbf{r}+\mathbf{R}) = u_{j,\mathbf{q}}(\mathbf{r})$

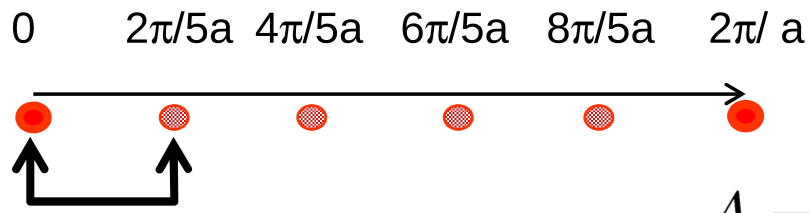
Exemplo: Teorema de Bloch em 1D.

- Rede direta (N=5):



$$L = 5a$$

- Rede recíproca: $\mathbf{a}_1 \cdot \mathbf{A}_1 = 2\pi$



$$k_1 = 2\pi/5a$$

$$A = 2\pi/a$$

$$\Psi_{m'}(x) = e^{iq_{m'}x}u_{m'}(x)$$

$$q_{m'} = \frac{2m'}{N}\left(\frac{\pi}{a}\right)$$

$$k_m = \frac{m}{N}\left(\frac{2\pi}{a}\right)$$

$$|2m'| \leq N$$

$$u_{m'}(x) = \sum_{n=-5}^{5} \mathcal{C}_{m'-n} e^{-i\frac{2\pi n}{a}x}$$

$$G = n\left(\frac{2\pi}{a}\right)$$

$$u_{m'}(x+a) = \sum_{n=-5}^{5} \mathcal{C}_{m'-n} e^{-i\frac{2\pi n}{a}x} e^{-i2\pi n} = u_{m'}(x)$$